Invariant theoretic approach to uncertainty relations for quantum systems

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Abstract

We present a general framework and procedure to derive uncertainty relations for observables of quantum systems in a covariant manner. All such relations are consequences of the positive semidefiniteness of the density matrix of a general quantum state. Particular emphasis is given to the action of unitary symmetry operations of the system on the chosen observables, and the covariance of the uncertainty relations under these operations. The general method is applied to the case of an n-mode system to recover the $Sp(2n, R)$-covariant multi mode generalization of the single mode Schrödinger-Robertson Uncertainty Principle; and to the set of all polynomials in canonical variables for a single mode system. In the latter situation, the case of the fourth order moments is analyzed in detail, exploiting covariance under the homogeneous Lorentz group $SO(2, 1)$ of which the symplectic group $Sp(2, R)$ is the double cover.

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I. INTRODUCTION

It is a well known historical fact that the $1925-1926$ discoveries of two equivalent mathematical formulations of quantum mechanics—Heisenberg's matrix form followed by Schrödinger's wave mechanical form—preceded the development of a physical interpretation of these formalisms [1]. The first important ingredient of the conventional interpretation was Born's 1926 identification of the squared modulus of a complex Schrödinger wavefunction as a probability [2]. The second ingredient developed in 1927 was Heisenberg's Uncertainty Principle (UP) [3]. To these may be added Bohr's Complementarity Principle which has a more philosophical flavour [4].

Heisenberg's original derivation of his position-momentum UP combined the formula for the resolving power of an optical microscope extrapolated to a hypothetical gamma ray microscope, with the energy and momentum relations for a single photon, in analysing the inherent limitations in simultaneous determinations of the position and momentum of an electron. His result indicated the limits of applicability of classical notions, in particular the spatial orbit of a point particle, in quantum mechanics.

More formal mathematical derivations of the UP, using the Born probability interpretation, soon followed. Prominent among them are the treatments of Kennard, Schrödinger, and Robertson [5]. Such a derivation was also presented by Heisenberg in his 1930 Chicago lectures [6].

The Heisenberg position-momentum UP is basically kinematical in nature. In contrast, the Bohr UP for time and energy involves quantum dynamics in an essential manner [7]. Later work on the UP has introduced a wide variety of ideas [8] and interpretations of the fluctuations or the uncertainties involved [9], such as in entropic [10] and other formulations [11].

Even for a one-dimensional quantum system, the Schrödinger-Robertson form of the UP displays more invariance than the Heisenberg form. Thus while the latter is invariant only under reciprocal scalings of position and momentum, and their interchange amounting to Fourier transformation, the former is invariant under the three-parameter Lie group $Sp(2, R)$ of linear canonical transformations. Fourier transformation, as well as reciprocal scalings, belong to $Sp(2, R)$ [12]. The generalisation of the Schrödinger-Robertson UP to any finite number, n, of degrees of freedom displays invariance under the group $Sp(2n, R)$ [13].

The purpose of this paper is to outline an invariant theoretic approach to general uncertainty relations for quantum systems. It combines a recapitulation and reexpression of some past results [14] with some new ones geared to practical applications. The analysis throughout is in the spirit of the Schrödinger-Robertson treatment, and, in particular, our considerations do not cover the entropic type uncertainty relations. All our considerations will be kinematical in nature.

The material of this paper is presented as follows. Section II sets up a general framework and procedure for deriving consequences of the positive semidefiniteness of the density matrix of a general quantum state, for the expectation values and fluctuations of a chosen (linearly independent) set of observables for the system. This has the form of a general uncertainty relation. A natural way to separate the expressions entering it into a symmetric fluctuation part, and an antisymmetric part contributed by commutators among the observables, hence specifically quantum in origin, is described. With respect to any unitary symmetry operation associated with the system, under which the chosen observables transform in a suitable manner, the uncertainty relation is shown to transform covariantly and to be preserved in content. In Section III this general framework is applied to the case of a quantum system involving n Cartesian canonical Heisenberg pairs, i.e., an n-mode system; and to the fluctuations in canonical 'coordinates' and 'momenta' in any state. The resulting n-mode generalization of the original Schrödinger-Robertson UP is seen to be explicitly covariant under the group $Sp(2n, R)$ of linear homogeneous canonical transformations. Section IV returns to the single mode system, but considers as the system of observables the infinite set of operator polynomials of all orders in the two canonical variables. The treatment is formal to the extent that unbounded operators are involved. An important role is played by the set of all finite-dimensional real nonunitary irreducible representations of the covariance group $Sp(2, R)$. We follow in spirit the structure of the basic theorems in the classical theory of moments. Thus the formal infinite-dimensional matrix uncertainty relation is reduced to a nested sequence of finite-dimensional requirements, of steadily increasing dimensions. While this case has been treated elsewhere [14], some of the subtler aspects are now carefully brought out. In this and the subsequent Sections the method of Wigner distributions is used as an extremely convenient technical tool. Section V treats in more detail the uncertainty relations of Section IV that go one step beyond the original Schrödinger-Robertson UP. Here all the fourth order moments of the canonical variables in a general state are involved. Their

fully covariant treatment brings in the defining and some other low dimensional represen-
tations of the three-dimensional Lorentz group $SO(2, 1)$. It is shown that the uncertainty
relations (to the concerned order) are all expressible in terms of $SO(2, 1)$ invariants. In
Section VI we describe an interesting aspect of the Schrödinger-Robertson UP in the light of
three-dimensional Lorentz geometry, which becomes particularly apparent through the use
of Wigner distribution methods. We argue that this should generalise to the conditions on
fourth (and higher) order moments as well. The paper ends with some concluding remarks
in Section VII.

II.   GENERAL FRAMEWORK

We consider a quantum system with associated Hilbert space $\mathcal{H}$, state vectors $|\psi\rangle$, $|\phi\rangle$,
$\cdots$ and inner product $\langle\phi|\psi\rangle$ as usual. A general (mixed) state is determined by a density
operator or density matrix $\hat{\rho}$ acting on $\mathcal{H}$ and obeying

$$\hat{\rho}^{\dagger} = \hat{\rho} \geq 0, \quad \text{Tr}\,\hat{\rho} = 1. \tag{2.1}$$

Then $\text{Tr}\,\hat{\rho}^2 = 1$ or < 1 distinguishes between pure and mixed states. Any hermitian observ-
able $\hat{A}$ of the system possesses the expectation value

$$\langle\hat{A}\rangle = \text{Tr}\,(\hat{\rho}\,\hat{A}) \tag{2.2}$$

in the state $\hat{\rho}$, the dependence of the left hand side on $\hat{\rho}$ being generally left implicit.

We now set up a general method which allows the drawing out of the consequences of the
nonnegativity of $\hat{\rho}$ in a systematic manner. This along with two elementary lemmas will be
the basis of our considerations.

Let $\hat{A}_a$, $a = 1, 2, \cdots, N$ be a set of N $linearly$ independent $hermitian$ operators, each
representing some observable of the system. We set up two formal N-component and $(N+1)$-
component column vectors with hermitian operator entries as follows:

$$\hat{A} = \begin{pmatrix} \hat{A}_1 \\ \vdots \\ \vdots \\ \hat{A}_N \end{pmatrix}, \quad \hat{\mathcal{A}} = \begin{pmatrix} 1 \\ \hat{A} \end{pmatrix} = \begin{pmatrix} 1 \\ \hat{A}_1 \\ \vdots \\ \vdots \\ \hat{A}_N \end{pmatrix}, \tag{2.3}$$

From $\hat{\mathcal{A}}$ we construct a square $(N+1)$-dimensional 'matrix' with operator entries as

$$\hat{\Omega} = \hat{\mathcal{A}}\hat{\mathcal{A}}^T = \begin{pmatrix} 1 & \cdots & \cdots & \hat{A}_b & \cdots \\ \vdots & & & \vdots & \\ \hat{A}_a & \cdots & \cdots & \hat{A}_a\hat{A}_b & \cdots \\ \vdots & & & \vdots & \end{pmatrix}. \tag{2.4}$$

Since $(\hat{A}_a\hat{A}_b)^\dagger = \hat{A}_b\hat{A}_a$, $\hat{\Omega}$ is 'hermitian' in the following sense: taking the operator hermitian conjugate of each element and then transposing the rows and columns leaves $\hat{\Omega}$ unchanged. In a state $\hat{\rho}$ we then have an $(N+1)$-dimensional numerical hermitian matrix Ω of the expectation values of the elements of $\hat{\Omega}$:

$$\Omega = \langle\hat{\Omega}\rangle = \mathrm{Tr}(\hat{\rho}\,\hat{\Omega}) = \begin{pmatrix} 1 & \cdots & \cdots & \langle\hat{A}_b\rangle & \cdots \\ \vdots & & & \vdots & \\ \langle\hat{A}_a\rangle & \cdots & \cdots & \langle\hat{A}_a\hat{A}_b\rangle & \cdots \\ \vdots & & & \vdots & \end{pmatrix},$$

i.e., $\Omega_{ab} = \mathrm{Tr}(\hat{\rho}\,\hat{\Omega}_{ab})$;

$$\Omega^\dagger = \Omega. \tag{2.5}$$

Now for any complex $(N+1)$ component column vector $\mathbf{C} = (c_0,\, c_1,\, \cdots,\, c_N)^T$ we have

$$\mathbf{C}^\dagger\,\hat{\Omega}\,\mathbf{C} = \mathbf{C}^\dagger\hat{\mathcal{A}}\,(\mathbf{C}^\dagger\hat{\mathcal{A}})^\dagger \geq 0,$$

$$\langle\mathbf{C}^\dagger\,\hat{\Omega}\,\mathbf{C}\rangle = \mathbf{C}^\dagger\,\Omega\,\mathbf{C} \geq 0, \tag{2.6}$$

leading immediately to:

Theorem 1 *Positivity of $\hat{\rho}$ imputes positivity to the matrix Ω, for every choice of $\hat{\mathcal{A}}$:*

$$\hat{\rho} \geq 0 \Rightarrow \Omega = \langle\hat{\Omega}\rangle = \mathrm{Tr}(\hat{\rho}\,\hat{\Omega}) \geq 0, \quad \forall\,\hat{\mathcal{A}}. \tag{2.7}$$

This is thus an uncertainty relation valid in every physical state $\hat{\rho}$.

Remark: It is for the sake of definiteness and keeping in view the ensuing applications that we have assumed the entries $\hat{A}_a$ of $\hat{\mathcal{A}}$ and $\hat{A}$ to be all hermitian. This can be relaxed and each $\hat{A}_a$ can be a general linear operator pertinent to the system. The only change would be the replacement of $\hat{\mathcal{A}}^T$ in Eq. (2.4) by $\hat{\mathcal{A}}^\dagger$, leading to a result similar to Theorem 1.

Depending on the basic kinematics of the system we can imagine various choices of the $\hat{A}_a$ geared to exhibiting corresponding symmetries or covariance properties of the uncertainty

relation (2.7). Specifically suppose there is a unitary operator $\overline{U}$ on $\mathcal{H}$ such that under conjugation the $\hat{A}_a$ go into (necessarily real) linear combinations of themselves:

$$\overline{U}\,\overline{U}^\dagger = \overline{U}^\dagger\,\overline{U} = \mathbb{1},$$

$$\overline{U}^{-1}\,\hat{A}_a\,\overline{U} = R_{ab}\,\hat{A}_b,$$

$$\overline{U}^{-1}\,\hat{\mathcal{A}}\,\overline{U} = \mathcal{R}\,\hat{\mathcal{A}},$$

$$\mathcal{R} = \begin{pmatrix} 1 & 0 \\ 0 & R \end{pmatrix}, \quad R = (R_{ab}). \tag{2.8}$$

The matrix R here is real N-dimensional nonsingular. Then combined with Eq. (2.5) we have:

$$\hat{\rho}' = \overline{U}\,\hat{\rho}\,\overline{U}^{-1} \Rightarrow \Omega' = \mathrm{Tr}(\hat{\rho}'\,\hat{\Omega}) = \mathrm{Tr}(\hat{\rho}\,\overline{U}^{-1}\,\hat{\mathcal{A}}\,\hat{\mathcal{A}}^T\,\overline{U})$$

$$= \mathcal{R}\,\Omega\,\mathcal{R}^T,$$

$$\Omega \geq 0 \Leftrightarrow \Omega' \geq 0. \tag{2.9}$$

This is because the passage $\Omega \to \Omega'$ is a congruence transformation. Thus the uncertainty relation (2.7) is covariant or explicitly preserved under the conjugation of the state $\hat{\rho}$ by the unitary transformation $\overline{U}$.

We now introduce two lemmas concerning (finite-dimensional) nonnegative matrices, whose proofs are elementary:

Lemma 1 *For a hermitian positive definite matrix in block form,*

$$Q = Q^\dagger = \begin{pmatrix} A & C^\dagger \\ C & B \end{pmatrix}, \quad A^\dagger = A, \quad B^\dagger = B, \tag{2.10}$$

we have

$$Q > 0 \Leftrightarrow A > 0 \text{ and } B - C\,A^{-1}C^\dagger > 0. \tag{2.11}$$

The proof consists in noting that by a congruence we can pass from Q to a block diagonal form [15]:

$$Q = \begin{pmatrix} \mathbb{1} & 0 \\ -CA^{-1} & \mathbb{1} \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & B - CA^{-1}C^\dagger \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ -CA^{-1} & \mathbb{1} \end{pmatrix}^\dagger. \tag{2.12}$$

Lemma 2 *If we separate a hermitian matrix Q into real symmetric and pure imaginary antisymmetric parts R, S then*

$$Q = Q^\dagger = R + iS \geq 0, \ \det S \neq 0 \Rightarrow R > 0. \tag{2.13}$$

The nonsingularity of S means that Q must be even dimensional. (The proof, which is elementary, is omitted).

Now we apply Lemma 1 to the $(N+1)$-dimensional matrix Ω in Eq. (2.5), choosing a partitioning where B is $N \times N$, C is $N \times 1$ and $C^\dagger$ is $1 \times N$:

$$\Omega = \begin{pmatrix} A & C^\dagger \\ C & B \end{pmatrix} : \ A = 1, \ B = (\langle \hat{A}_a \hat{A}_b \rangle), \ C = (\langle \hat{A}_a \rangle). \tag{2.14}$$

Then from Eq. (2.11) we conclude:

Theorem 2

$$\hat{\rho} \geq 0 \Rightarrow \Omega \geq 0 \Leftrightarrow$$
$$\tilde{\Omega} = (\langle (\hat{A}_a - \langle \hat{A}_a \rangle)(\hat{A}_b - \langle \hat{A}_b \rangle) \rangle) \geq 0. \tag{2.15}$$

All expectation values involved in the elements of the $N \times N$ matrix $\tilde{\Omega}$ are with respect to the state $\hat{\rho}$.

The motivation for the definitions of $\hat{\mathcal{A}}$, $\hat{\Omega}$ as in Eq. (2.3) is now clear: after an application of Lemma 1 we immediately descend from the matrix Ω to the matrix $\tilde{\Omega}$ involving only expectation values of products of deviations from means. It is then natural to write the elements of $\tilde{\Omega}$ as follows:

$$\Delta \hat{A}_a = \hat{A}_a - \langle \hat{A}_a \rangle,$$
$$\tilde{\Omega}_{ab} = \langle \Delta \hat{A}_a \Delta \hat{A}_b \rangle. \tag{2.16}$$

We revert to this form shortly.

The covariance of the statement (2.15), Theorem 2, under a unitary symmetry $\overline{U}$ acting as in Eq. (2.8) follows from a brief calculation:

$$\hat{\rho} \to \hat{\rho}' = \overline{U} \hat{\rho} \overline{U}^{-1} \Rightarrow$$
$$\overline{U}^{-1}(\hat{A}_a - \text{Tr}(\hat{\rho}' \hat{A}_a))\overline{U} = \overline{U}^{-1} \hat{A}_a \overline{U} - \text{Tr}(\hat{\rho} \overline{U}^{-1} \hat{A}_a \overline{U})$$
$$= R_{ab}(\hat{A}_b - \text{Tr}(\hat{\rho} \hat{A}_b));$$
$$\tilde{\Omega} \to \tilde{\Omega}' = R\tilde{\Omega}R^T;$$
$$\tilde{\Omega} \geq 0 \Leftrightarrow \tilde{\Omega}' \geq 0. \tag{2.17}$$

We now return to Eq. (2.16). The state $\hat{\rho}$ being kept fixed, we can split the hermitian $N \times N$ matrix $\tilde{\Omega}$ into real symmetric and pure imaginary antisymmetric parts as follows:

$$\tilde{\Omega}_{ab} = V_{ab}(\hat{\rho}\,;\,\hat{A}) + \frac{i}{2}\,\omega_{ab}(\hat{\rho}\,;\,\hat{A}),$$

$$V_{ab}(\hat{\rho}\,;\,\hat{A}) = V_{ba}(\hat{\rho}\,;\,\hat{A}) = \frac{1}{2}\langle\{\Delta\hat{A}_a,\,\Delta\hat{A}_b\}\rangle$$

$$= \frac{1}{2}\langle\{\hat{A}_a,\,\hat{A}_b\}\rangle - \langle\hat{A}_a\rangle\langle\hat{A}_b\rangle;$$

$$\omega_{ab}(\hat{\rho}\,;\,\hat{A}) = -\omega_{ba}(\hat{\rho}\,;\,\hat{A}) = -\,i\,\langle[\hat{A}_a,\,\hat{A}_b]\rangle. \tag{2.18}$$

The brackets $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ denote, as usual, the commutator and anticommutator respectively. The natural physical identification of the $N \times N$ real symmetric matrix $V(\hat{\rho}\,;\,\hat{A}) = (V_{ab}(\hat{\rho}\,;\,\hat{A}))$ is that it is the variance matrix (or matrix of covariances) associated with the set $\{\hat{A}_a\}$ in the state $\hat{\rho}$. The uncertainty relation (2.15) now reads:

$$\hat{\rho} \geq 0 \ \Rightarrow \ V(\hat{\rho}\,;\,\hat{A}) + \frac{i}{2}\,\omega(\hat{\rho}\,;\,\hat{A}) \geq 0, \tag{2.19}$$

and then by Lemma 2 we have the possible further consequence:

$$\det\omega(\hat{\rho}\,;\,\hat{A}) \neq 0 \Rightarrow V(\hat{\rho}\,;\,\hat{A}) > 0\,. \tag{2.20}$$

Remark: In case the operators $\hat{A}_a$ commute pairwise, in any state $\hat{\rho}$ there is a 'classical' joint probability distribution over the sets of simultaneous eigenvalues of all the $\hat{A}_a$. In such a case, the term ω in Eqs. (2.18, 2.19) vanishes identically, and the uncertainty relation (2.19) is a 'classical' statement [16]. Therefore in the general case a good name for $\omega_{ab}(\hat{\rho}\,;\,\hat{A})$ is that it is the 'commutator correction' term.

It is instructive to appreciate that while the original definitions of Ω and $\tilde{\Omega}$, starting from the operator sets $\hat{\mathcal{A}}$ and $\hat{\Omega}$, make it essentially trivial to see that they must be nonnegative, the form (2.19) of the general uncertainty relation gives prominence to the variance matrix $V(\hat{\rho}\,;\,\hat{A})$. In addition, as seen earlier, the matrix Ω does not directly deal with fluctuations. It is after the use of Lemma 1 that we obtain the matrix $\tilde{\Omega}$ involving the fluctuations.

From Eqs. (2.8, 2.17), the effect of a unitary symmetry transformation on the real matrices $V(\hat{\rho}\,;\,\hat{A})$ and $\omega(\hat{\rho}\,;\,\hat{A})$ is seen to be:

$$\hat{\rho}' = \overline{U}\,\hat{\rho}\,\overline{U}^{-1} \ :\ V(\hat{\rho}'\,;\,\hat{A}) = R\,V(\hat{\rho}\,;\,\hat{A})\,R^T,$$

$$\omega(\hat{\rho}'\,;\,\hat{A}) = R\,\omega(\hat{\rho}\,;\,\hat{A})\,R^T, \tag{2.21}$$

so that the form (2.19) of the uncertainty relation is manifestly preserved.

In later work, when there is no danger of confusion, we sometimes omit the arguments $\hat{\rho}$ and $\hat{A}$ in V and ω.

III.   THE MULTI MODE SCHRÖDINGER-ROBERTSON UNCERTAINTY PRINCIPLE

As a first example of the general framework we consider briefly the Schrödinger-Robertson UP for an n-mode system, which has been extensively discussed elsewhere [13, 17].

The basic operators, Cartesian coordinates and momenta, consist of n pairs of canonical $\hat{q}$ and $\hat{p}$ variables obeying the Heisenberg canonical commutation relations. The operator properties and relations are:

$$a = 1,\, 2,\, \cdots,\, 2n\,:\quad \hat{\xi}_a = \begin{cases} \hat{q}_{(a+1)/2}, & a \text{ odd}, \\ \hat{p}_{a/2}, & a \text{ even}; \end{cases}$$

$$\hat{\xi}_a^\dagger = \hat{\xi}_a\,;$$

$$\left[\hat{\xi}_a,\, \hat{\xi}_b\right] = i\hbar \beta_{ab}\,,$$

$$\beta = \text{block diag}\,(\,i\sigma_2,\, i\sigma_2,\, \cdots,\, i\sigma_2\,) = \mathbb{1}_{n \times n} \otimes i\sigma_2\,. \tag{3.1}$$

These operators act irreducibly on the system Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$.

We take these $\hat{\xi}_a$ as the $\hat{A}_a$ of Eq. (2.3), so here $N = 2n$:

$$\hat{\mathcal{A}} \to \begin{pmatrix} 1 \\ \hat{\xi} \end{pmatrix},\quad \hat{A} \to \hat{\xi} = \begin{pmatrix} \hat{\xi}_1 \\ \vdots \\ \hat{\xi}_{2n} \end{pmatrix} = \begin{pmatrix} \hat{q}_1 \\ \hat{p}_1 \\ \vdots \\ \hat{q}_n \\ \hat{p}_n \end{pmatrix}. \tag{3.2}$$

Then for any state $\hat{\rho}$, the variance matrix V has elements

$$V_{ab} = \frac{1}{2}\,\text{Tr}\left(\hat{\rho}\,\{\hat{\xi}_a - \text{Tr}(\hat{\rho}\,\hat{\xi}_a),\, \hat{\xi}_b - \text{Tr}(\hat{\rho}\,\hat{\xi}_b)\}\right)$$

$$= \frac{1}{2}\langle\{\hat{\xi}_a,\, \hat{\xi}_b\}\rangle - \langle\hat{\xi}_a\rangle\,\langle\hat{\xi}_b\rangle, \tag{3.3}$$

while the antisymmetric matrix ω is just the *state-independent* numerical 'symplectic metric matrix' β:

$$\omega_{ab} = -i\,\langle\left[\hat{\xi}_a,\, \hat{\xi}_b\right]\rangle = \hbar \beta_{ab}. \tag{3.4}$$

The uncertainty relation (2.19) then becomes the n-mode Schrödinger-Robertson UP:

$$\hat{\rho} \geq 0 \Rightarrow V + i\frac{\hbar}{2}\beta \geq 0 \ (\Rightarrow V > 0), \tag{3.5}$$

the second step following from Eq. (2.20) as β is nonsingular.

For $n = 1$, a single mode, the matrices V and β are two-dimensional:

$$V = \begin{pmatrix} (\Delta q)^2 & \Delta(q, p) \\ \Delta(q, p) & (\Delta p)^2 \end{pmatrix},$$

$$(\Delta q)^2 = \langle(\hat{q} - \langle\hat{q}\rangle)^2\rangle, \quad (\Delta p)^2 = \langle(\hat{p} - \langle\hat{p}\rangle)^2\rangle,$$

$$\Delta(q, p) = \frac{1}{2}\langle\{\hat{q} - \langle\hat{q}\rangle, \hat{p} - \langle\hat{p}\rangle\}\rangle;$$

$$\beta = i\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{3.6}$$

Then (3.5) simplifies to

$$\begin{pmatrix} (\Delta q)^2 & \Delta(q, p) + \frac{i}{2}\hbar \\ \Delta(q, p) - \frac{i}{2}\hbar & (\Delta p)^2 \end{pmatrix} \geq 0,$$

$$i.e., \ \det\left(V + \frac{i}{2}\hbar\beta\right) \equiv (\Delta q)^2(\Delta p)^2 - (\Delta(q, p))^2 - \frac{\hbar^2}{4} \geq 0,$$

$$i.e., \ \det V \geq \frac{\hbar^2}{4}, \tag{3.7}$$

the original Schrödinger-Robertson UP.

Returning to n modes, the $Sp(2n, R)$ covariance of the Schrödinger-Robertson UP (3.5) takes the following form: If $S \in Sp(2n, R)$, i.e., any real $2n \times 2n$ matrix obeying $S\beta S^T = \beta$, then the new operators

$$\hat{\xi}'_a = S_{ab}\,\hat{\xi}_b \tag{3.8}$$

preserve the commutation relations in Eq. (3.1) and hence are unitarily related to the $\hat{\xi}_a$. These unitary transformations constitute the double valued metaplectic unitary representation of $Sp(2n, R)$ [18]:

$$S \in Sp(2n, R) \rightarrow \overline{U}(S) = \text{unitary operator on } \mathcal{H},$$

$$\overline{U}(S')\overline{U}(S) = \pm\overline{U}(S'S);$$

$$\overline{U}(S)^{-1}\,\hat{\xi}_a\,\overline{U}(S) = S_{ab}\,\hat{\xi}_b. \tag{3.9}$$

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Then, as an instance of Eqs. (2.21) we have the results:

$$\hat{\rho} \to \hat{\rho}' = \overline{U}(S)\,\hat{\rho}\,\overline{U}(S)^{-1} \Rightarrow V \to V' = S\,V\,S^T,$$

$$V + \frac{i}{2}\,\hbar\,\beta \geq 0 \iff V' + \frac{i}{2}\,\hbar\,\beta \geq 0. \tag{3.10}$$

Remark: The n-mode Schrödinger-Robertson UP (3.5), with its explicit $Sp(2n,\,R)$ co-variance (3.10), constitutes the answer to an important question raised by Littlejohn [19]: under what conditions is a real normalized Gaussian function on a $2n$-dimensional phase space the Wigner distribution for some quantum state? The answer is stated in terms of the variance matrix which of course determines the Gaussian up to phase space displacements [And these phase space displacements have no role to play on the 'Wigner quality' of a phase space distribution]. This result has been used extensively in both classical and quantum optics [17], and more recently in quantum information theory of continuous variable canonical systems [20].

As a last comment we mention that as according to Eq. (3.5) the variance matrix V is always positive definite, by Williamson's celebrated theorem an $S \in Sp(2n,\,R)$ can be found such that V' in Eq. (3.10) becomes diagonal [21, 22]. In general, though, the diagonal elements of V' will not be the eigenvalues of V.

IV. HIGHER ORDER MOMENTS FOR SINGLE MODE SYSTEM

We now revert to the $n = 1$ case of one canonical pair of hermitian operators $\hat{q}$ and $\hat{p}$, but consider expectation values of expressions in these operators of order greater than two. The relevant Hilbert space is of course $\mathcal{H} = L^2(\mathbb{R})$. As a useful computational tool we work with the Wigner distribution description of quantum states, and the associated Weyl rule of association of (hermitian) operators with (real) classical phase space functions.

Given a quantum mechanical state $\hat{\rho}$, the corresponding Wigner distribution is a function on the classical two-dimensional phase space:

$$W(q,p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dq' \left\langle q - \frac{1}{2}q' \left| \hat{\rho} \right| q + \frac{1}{2}q' \right\rangle e^{ipq'/\hbar}. \tag{4.1}$$

Thus it is a partial Fourier transform of the position space matrix elements of $\hat{\rho}$. This

function is real and normalised to unity, but need not be pointwise nonnegative:

$$\hat{\rho}^\dagger = \hat{\rho} \Rightarrow W(q,p)^* = W(q,p)\,;$$
$$\mathrm{Tr}\,\hat{\rho} = 1 \Rightarrow \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dqdp\, W(q,p) = 1. \tag{4.2}$$

The operator $\hat{\rho}$ and the function $W(q,p)$ determine each other uniquely. The *key property* is that the quantum expectation values of operator exponentials are equal to the classical phase space averages of classical exponentials with respect to $W(q,p)$ [23]:

$$\mathrm{Tr}(\hat{\rho}\,e^{i(\theta\,\hat{q}-\tau\,\hat{p})}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dqdp\, W(q,p)e^{i(\theta\,q-\tau\,p)}, \quad -\infty < \theta,\tau < \infty. \tag{4.3}$$

By expanding the exponentials and comparing powers of θ and τ we get:

$$\mathrm{Tr}(\hat{\rho}\,\widehat{(q^n\,p^{n'})}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dqdp\, W(q,p)q^n p^{n'},$$
$$\widehat{(q^n\,p^{n'})} = \text{coefficient of } \frac{(i\theta)^n}{n!}\frac{(-i\tau)^{n'}}{n'!} \text{ in } e^{i(\theta\,\hat{q}-\tau\,\hat{p})}$$
$$= \frac{n!\,n'!}{(n+n')!} \times \text{ coefficient of } \theta^n(-\tau)^{n'} \text{ in } (\theta\,\hat{q}-\tau\,\hat{p})^{n+n'},$$
$$n,\,n' = 0,\,1,\,2,\,\cdots. \tag{4.4}$$

Thus $\widehat{(q^n\,p^{n'})}$ is an hermitian operator polynomial in $\hat{q}$ and $\hat{p}$ associated to the classical real monomial $q^n p^{n'}$. This is the Weyl rule of association indicated by

$$\widehat{(q^n\,p^{n'})} = (q^n\,p^{n'})_W, \tag{4.5}$$

so Eq. (4.4) appears as

$$\mathrm{Tr}(\hat{\rho}\,(q^n\,p^{n'})_W) = \int\int dqdp\, W(q,p)\,q^n p^{n'}. \tag{4.6}$$

We regard the polynomials $(q^n\,p^{n'})_W$ as the basic 'quantum monomials'. By linearity the association (4.5) can be extended to general functions on the classical phase space, leading to the scheme:

$$f(q,p) = \text{real classical function} \rightarrow \hat{F} = (f(q,p))_W = \text{hermitian operator on } \mathcal{H},$$
$$\mathrm{Tr}(\hat{\rho}\,\hat{F}) = \int\int dqdp\, W(q,p)\,f(q,p). \tag{4.7}$$

Remarks: Two useful comments may be made at this point. For any pair of states $\hat{\rho}$, $\hat{\rho}'$ we have

$$\mathrm{Tr}(\hat{\rho}\,\hat{\rho}') = \int\int dqdp\, W(q,p)\,W'(q,p) \geq 0. \tag{4.8}$$

Based on this, one can see the following: a given real normalised phase space function $W(q,p)$ is a Wigner distribution (corresponding to some physical state $\hat{\rho}$) if and only if the overlap integral on the right hand side of Eq. (4.8) is nonnegative for all Wigner distributions $W'(q,p)$. Secondly, we refer to the remarks made following Eq. (2.20) concerning the commutative case $\left[\hat{A}_a,\ \hat{A}_b\right] = 0$. This happens for instance when $\hat{A}_a = f_a(\hat{q})$ for all a. In that case, only the integral of $W(q,p)$ over p is relevant, and this is known to be the coordinate space probability density in the state $\hat{\rho}$ [24]. In the multi mode case this generalizes to the following statement: the result of integrating $W(q_1, p_1, q_2, p_2, \cdots, q_n, p_n)$ over any (n-dimensional) linear Lagrangian subspace in phase space is always a genuine probability distribution (the marginal) over the 'remaining' n phase space variables. *This marginal is basically the squared modulus, or probability density in the Born sense, of a wavefunction on the corresponding 'configuration space', generalised to the case of a mixed state* [24].

The covariance group of the canonical commutation relation obeyed by $\hat{q}$ and $\hat{p}$ is (apart from phase space translations) the group $Sp(2,\ R)$:

$$Sp(2,\ R) = \left\{ S = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \text{real } 2 \times 2 \text{ matrix} \mid S\,\sigma_2\,S^T = \sigma_2,\ \text{i.e., } \det S = 1 \right\}. \quad (4.9)$$

The actions on $\hat{q}$ and $\hat{p}$ by matrices and by the unitary metaplectic representation of $Sp(2,\ R)$ are connected in this manner:

$$S \in Sp(2,\ R) \to \overline{U}(S) = \text{unitary operator on } \mathcal{H}\,;$$
$$\xi = \begin{pmatrix} q \\ p \end{pmatrix} \to \hat{\xi} = (\xi)_W = \begin{pmatrix} \hat{q} \\ \hat{p} \end{pmatrix}\,:$$
$$\overline{U}(S)^{-1}\,\hat{\xi}\,\overline{U}(S) = S\,\hat{\xi}. \quad (4.10)$$

The effect on $W(q,p) \equiv W(\xi)$ is then given as [13, 17]:

$$\hat{\rho}' = \overline{U}(S)\,\hat{\rho}\,\overline{U}(S)^{-1} \leftrightarrow W'(\xi) = W(S^{-1}\,\xi). \quad (4.11)$$

We now introduce a more suggestive notation for the classical monomials $q^n p^{n'}$ and their operator counterparts $(q^n p^{n'})_W$. This is taken from the quantum theory of angular momentum (QTAM) and uses the fact that finite-dimensional nonunitary irreducible real representations of $Sp(2,\ R)$ are related to the unitary irreducible representations of $SU(2)$ by analytic continuation. (Indeed the two sets of generators are related by the unitary Weyl

trick). We use 'quantum numbers' $j = 0, \frac{1}{2}, 1, \cdots, m = j, j-1, \cdots, -j$ as in QTAM and define the hermitian monomial basis for operators on $\mathcal{H}$ in this way:

$$\hat{T}_{jm} = (q^{j+m}p^{j-m})_W = \text{coefficient of } \frac{(2j)!}{(j+m)!(j-m)!}\,\theta^{j+m}(-\tau)^{j-m} \text{ in } (\theta\,\hat{q} - \tau\,\hat{p})^{2j},$$

$$j = 0, \frac{1}{2}, 1, \cdots, ; \quad m = j, j-1, \cdots, -j. \tag{4.12}$$

For the first few values of j we have

$$(\hat{T}_{\frac{1}{2}m}) = \begin{pmatrix} \hat{q} \\ \hat{p} \end{pmatrix}; \quad (\hat{T}_{1m}) = \begin{pmatrix} \hat{q}^2 \\ \frac{1}{2}\{\hat{q}, \hat{p}\} \\ \hat{p}^2 \end{pmatrix}; \quad (\hat{T}_{\frac{3}{2}m}) = \begin{pmatrix} \hat{q}^3 \\ \frac{1}{3}(\hat{q}^2\hat{p} + \hat{q}\hat{p}\hat{q} + \hat{p}\hat{q}^2) \\ \frac{1}{3}(\hat{q}\hat{p}^2 + \hat{p}\hat{q}\hat{p} + \hat{p}^2\hat{q}) \\ \hat{p}^3 \end{pmatrix};$$

$$(\hat{T}_{2m}) = \begin{pmatrix} \hat{q}^4 \\ \frac{1}{4}(\hat{q}^3\hat{p} + \hat{q}^2\hat{p}\hat{q} + \hat{q}\hat{p}\hat{q}^2 + \hat{p}\hat{q}^3) \\ \frac{1}{6}(\hat{q}^2\hat{p}^2 + \hat{q}\hat{p}\hat{q}\hat{p} + \hat{q}\hat{p}^2\hat{q} + \hat{p}\hat{q}^2\hat{p} + \hat{p}\hat{q}\hat{p}\hat{q} + \hat{p}^2\hat{q}^2) \\ \frac{1}{4}(\hat{q}\hat{p}^3 + \hat{p}\hat{q}\hat{p}^2 + \hat{p}^2\hat{q}\hat{p} + \hat{p}^3\hat{q}) \\ \hat{p}^4 \end{pmatrix}. \tag{4.13}$$

Then we have the consequences:

$$\text{Tr}(\hat{\rho}\,\hat{T}_{jm}) = \int\int dq dp\, W(q,p)\, q^{j+m}\, p^{j-m} \equiv \overline{q^{j+m}\, p^{j-m}};$$

$$S \in Sp(2, R): \quad \overline{U}(S)^{-1}\,\hat{T}_{jm}\,\overline{U}(S) = \sum_{m'=-j}^{j} K_{mm'}^{(j)}(S)\,\hat{T}_{jm'}. \tag{4.14}$$

The quantum expectation values of the $\hat{T}_{jm}$ are phase space moments of $W(q,p)$, denoted for convenience with an overhead bar. The matrices $K^{(j)}(S)$ constitute the $(2j+1)$-dimensional real nonunitary irreducible representation of $Sp(2, R)$ obtained from the familiar 'spin j' unitary irreducible representation of $SU(2)$ by analytic continuation. For $j = \frac{1}{2}$, we have $K^{(1/2)}(S) = S$. The representation $K^{(1)}(S)$ corresponding to $j = 1$ will be seen to engage our sole attention in Section V.

The noncommutative (but associative) product law for the hermitian monomial operators $\hat{T}_{jm}$ has an interesting form, being essentially determined by the $SU(2)$ Clebsch-Gordan coefficients. This is not surprising, in view of the connection between $SU(2)$ and $Sp(2, R)$ representations (in finite dimensions) mentioned above. In fact for these representations and in chosen bases, $SU(2)$ and $Sp(2, R)$ share the same Clebsch-Gordan coefficients [14].

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The product formula has a particularly simple structure if we (momentarily) use suitable numerical multiples of $\hat{T}_{jm}$:

$$\hat{\tau}_{jm} = \hat{T}_{jm}/\sqrt{(j+m)!(j-m)!}. \tag{4.15}$$

Then we find [14]

$$\hat{\tau}_{jm}\,\hat{\tau}_{j'm'} = \sum_{j''=|j-j'|}^{j+j'} \left(\frac{i\hbar}{2}\right)^{j+j'-j''} \sqrt{\frac{(j+j'+j''+1)!}{(2j''+1)(j+j'-j'')!(j'+j''-j)!(j''+j-j')!}}$$
$$\times C^{j\,j'\,j''}_{m\,m'\,m+m'}\,\hat{\tau}_{j'',\,m+m'}. \tag{4.16}$$

The $C^{j\,j'\,j''}_{m\,m'\,m''}$ are the $SU(2)$ Clebsch-Gordan coefficients familiar from QTAM [25]. We will use this product rule in the sequel.

Now we apply the general framework of Section II to the present situation. We will use a notation similar to that in the main theorems of the classical theory of moments. We take $\hat{A}$ and $\hat{\mathcal{A}}$ to formally be infinite component column vectors with hermitian entries:

$$\hat{A} = \begin{pmatrix} \vdots \\ \hat{T}_{jm} \\ \vdots \end{pmatrix} = (\hat{T}_{\frac{1}{2}\,\frac{1}{2}},\, \hat{T}_{\frac{1}{2}\,\frac{-1}{2}},\, \hat{T}_{1\,1},\, \hat{T}_{1\,0},\, \hat{T}_{1\,-1},\, \cdots,\, \hat{T}_{jj},\, \cdots,\, \hat{T}_{j,-j},\, \cdots)^{T},$$

$$\hat{\mathcal{A}} = \begin{pmatrix} 1 \\ \hat{A} \end{pmatrix}. \tag{4.17}$$

Thus the subscript a of Eq. (2.4) is now the pair jm taking values in the sequence given above. To simplify notation, as $\hat{A}$ is kept fixed, we will not indicate it as an argument in various quantities. The general entries in the infinite-dimensional matrices $\hat{\Omega}$, Ω, $\tilde{\Omega}$ in Eqs. (2.4, 2.5) are then:

$$\hat{\Omega}_{jm,j'm'} = \hat{T}_{jm}\,\hat{T}_{j'm'}\,;$$
$$\Omega_{jm,j'm'}(\hat{\rho}) = \mathrm{Tr}(\hat{\rho}\,\hat{T}_{jm}\,\hat{T}_{j'm'}) = \langle \hat{T}_{jm}\,\hat{T}_{j'm'}\rangle\,;$$
$$\tilde{\Omega}_{jm,j'm'}(\hat{\rho}) = \langle(\hat{T}_{jm} - \langle\hat{T}_{jm}\rangle)\,(\hat{T}_{j'm'} - \langle\hat{T}_{j'm'}\rangle)\rangle. \tag{4.18}$$

(In $\hat{\Omega}$ and Ω, for $j = m = 0$, we have $\hat{T}_{00} = 1$). By using the product rule (4.16) the (generally nonhermitian) operator $\hat{T}_{jm}\,\hat{T}_{j'm'}$ can be written as a complex linear combination of $\hat{T}_{j'',m+m'}$ with $j'' = j+j', j+j'-1, \cdots, |j-j'|$. The variance matrix $V(\hat{\rho})$ in Eq. (2.18) has the elements

$$V_{jm,j'm'}(\hat{\rho}) = \frac{1}{2}\langle\{\hat{T}_{jm},\,\hat{T}_{j'm'}\}\rangle - \langle\hat{T}_{jm}\rangle\,\langle\hat{T}_{j'm'}\rangle. \tag{4.19}$$

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From the known symmetry relation [25]

$$C^{j'\,j\,j''}_{m'\,m\,m+m'} = (-1)^{j+j'-j''}\, C^{j\,j'\,j''}_{m\,m'\,m+m'} \tag{4.20}$$

we see that in the anticommutator term in Eq. (4.19) only $\hat{T}^{j''}_{m+m'}$ for $j'' = j+j'$, $j+j' - 2$, $j+j'-4$, $\cdots$ will appear with real coefficients. On the other hand, for the antisymmetric part ω_{ab} of Eq. (2.18) we have

$$\omega_{jm,j'm'}(\hat{\rho}) = -i\left\langle \left[\hat{T}_{jm},\, \hat{T}_{j'm'}\right]\right\rangle, \tag{4.21}$$

so now by Eq. (4.20) the commutator here is a linear combination of terms $\hat{T}^{j''}_{m+m'}$ for $j'' = j + j' - 1$, $j + j' - 3$, $\cdots$ with pure imaginary coefficients. There is, therefore, a clean separation of the product $\hat{T}_{jm}\,\hat{T}_{j'm'}$ into a hermitian part in V and an antihermitian part in ω. With these facts in mind, the uncertainty relation (2.19) is in hand:

$$V_{jm,j'm'}(\hat{\rho}) = \sum_{j+j'-j''\ \text{even}} \cdots \langle \hat{T}_{j'',m+m'}\rangle - \langle \hat{T}_{jm}\rangle\,\langle \hat{T}_{j'm'}\rangle,$$

$$\omega_{jm,j'm'}(\hat{\rho}) = \sum_{j+j'-j''\ \text{odd}} \cdots \langle \hat{T}_{j'',m+m'}\rangle\,;$$

$$(\tilde{\Omega}_{jm,j'm'}(\hat{\rho})) = (V_{jm,j'm'}(\hat{\rho})) + \frac{i}{2}\,(\omega_{jm,j'm'}(\hat{\rho})) \geq 0. \tag{4.22}$$

Each matrix element of $V(\hat{\rho})$ (apart from the subtracted term) and of $\omega(\rho)$ appears as some real linear combination of expectation values of hermitian monomial operators, i.e., of moments of $W(q,p)$; however, in this way of writing, the essentially trivial nature of the statement $\tilde{\Omega}(\hat{\rho}) \geq 0$ is not manifest.

The covariance group in this problem is of course $Sp(2,\,R)$. From Eq. (4.14) we see that under conjugation by the metaplectic group unitary operator $\overline{U}(S)$, the column vector $\hat{A}$ of Eq. (4.17) transforms as a direct sum of the sequence of finite-dimensional real irreducible nonunitary representation matrices $K^{(1/2)}(S) = S$, $K^{(1)}(S)$, $K^{(3/2)}(S) \cdots$; so Eq. (2.8) in the present context is [14]:

$$S \in Sp(2,\,R): \quad \overline{U}(S)^{-1}\,\hat{A}\,\overline{U}(S) = K(S)\,\hat{A},$$

$$K(S) = K^{(1/2)}(S) \oplus K^{(1)}(S) \oplus K^{(3/2)}(S) \oplus \cdots \tag{4.23}$$

From Eq. (2.21), when $\hat{\rho} \to \hat{\rho}' = \overline{U}(S)\,\hat{\rho}\,\overline{U}(S)^{-1}$ both $V(\hat{\rho})$ and $\omega(\hat{\rho})$ experience congruence transformations by $K(S)$, and the formal uncertainty relation (4.22) is preserved.

Up to this point the use of infinite component $\hat{A}$ and infinite-dimensional Ω, $\tilde{\Omega}$, V and ω has been formal. We may now interpret the uncertainty relation (4.22) in practical terms to mean that for each finite $N = 1, 2, \cdots$, the principal submatrix of $\tilde{\Omega}(\hat{\rho})$ formed by its first N rows and columns should be nonnegative. However, in order to maintain $Sp(2, R)$ covariance, a slight modification of this procedure is desirable. If for each $J = \frac{1}{2}, 1, \frac{3}{2}, \cdots$ we include all values of jm for $j \leq J$, the number of rows (and columns) involved is $N_J = J(2J + 3)$, the sequence of integers $2, 5, 9, 14, \cdots$. Let us then define hierarchies of N_J-dimensional matrices as:

$$J = \frac{1}{2}, 1, \frac{3}{2}, \cdots :$$
$$\tilde{\Omega}^{(J)}(\hat{\rho}) = (\tilde{\Omega}_{jm,j'm'}(\hat{\rho})),$$
$$V^{(J)}(\hat{\rho}) = (V_{jm,j'm'}(\hat{\rho})),$$
$$\omega^{(J)}(\hat{\rho}) = (\omega_{jm,j'm'}(\hat{\rho})), \;\; j, j' = \frac{1}{2}, 1, \cdots, J;$$
$$\tilde{\Omega}^{(J)}(\hat{\rho}) = V^{(J)}(\hat{\rho}) + \frac{i}{2}\omega^{(J)}(\hat{\rho}). \tag{4.24}$$

However, in each of these matrices *there is no J dependence in their matrix elements*. Each also naturally breaks up into blocks of dimension $(2j+1)(2j'+1)$ for each pair (j, j') present, and these can be denoted by $\tilde{\Omega}^{(j,j')}(\hat{\rho})$, $V^{(j,j')}(\hat{\rho})$, $\omega^{(j,j')}(\hat{\rho})$. Symbolically,

$$\tilde{\Omega}^{(J)}(\hat{\rho}) = \begin{pmatrix} & \vdots & \\ \cdots & \tilde{\Omega}^{(j,j')}(\hat{\rho}) & \cdots \\ & \vdots & \end{pmatrix} \tag{4.25}$$

and similary for $V^{(J)}(\hat{\rho})$ and $\omega^{(J)}(\hat{\rho})$. As examples we have:

$$\tilde{\Omega}^{(1/2)}(\hat{\rho}) = (\tilde{\Omega}^{(\frac{1}{2},\frac{1}{2})}(\hat{\rho}));$$
$$\tilde{\Omega}^{(1)}(\hat{\rho}) = \begin{pmatrix} \tilde{\Omega}^{(\frac{1}{2},\frac{1}{2})}(\hat{\rho}) & \tilde{\Omega}^{(\frac{1}{2},1)}(\hat{\rho}) \\ \tilde{\Omega}^{(1,\frac{1}{2})}(\hat{\rho}) & \tilde{\Omega}^{(1,1)}(\hat{\rho}) \end{pmatrix}, \tag{4.26}$$

and correspondingly for $V^{(J)}$, $\omega^{(J)}$. Moreover, in going from J to $J + \frac{1}{2}$, we have an augmentation of each matrix with $2(J + 1)$ new rows and columns,

$$\tilde{\Omega}^{(J+1/2)}(\hat{\rho}) = \begin{pmatrix} & & & & & \vdots & \tilde{\Omega}^{(\frac{1}{2},J+\frac{1}{2})}(\hat{\rho}) \\ & & \tilde{\Omega}^{(J)}(\hat{\rho}) & & & \vdots & \vdots \\ & & & & & \vdots & \tilde{\Omega}^{(J,J+\frac{1}{2})}(\hat{\rho}) \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \tilde{\Omega}^{(J+\frac{1}{2},\frac{1}{2})}(\hat{\rho}) & \cdots & \tilde{\Omega}^{(J+\frac{1}{2},J)}(\hat{\rho}) & & \vdots & \tilde{\Omega}^{(J+\frac{1}{2},J+\frac{1}{2})}(\hat{\rho}) \end{pmatrix}. \tag{4.27}$$

The formal uncertainty relation (4.22) now translates into a hierarchy of finite-dimensional matrix conditions

$$\tilde{\Omega}^{(J)}(\hat{\rho}) = V^{(J)}(\hat{\rho}) + \frac{i}{2}\omega^{(J)}(\hat{\rho}) \geq 0, \ J = \frac{1}{2}, \ 1, \ \frac{3}{2}, \ \cdots . \tag{4.28}$$

(Of course, for a given state $\hat{\rho}$, moments may exist and be finite only up to some value $J_{\max}$ of J, so the hierarchy (4.28) also terminates at this point). The lowest condition in this hierarchy, $J = \frac{1}{2}$, takes us back to Eqs. (3.6, 3.7):

$$\tilde{\Omega}^{\left(\frac{1}{2}\right)}(\hat{\rho}) = \tilde{\Omega}^{\left(\frac{1}{2},\frac{1}{2}\right)}(\hat{\rho}) = V^{\left(\frac{1}{2}\right)}(\hat{\rho}) + \frac{i}{2}\omega^{\left(\frac{1}{2}\right)}(\hat{\rho}) ;$$

$$V^{\left(\frac{1}{2}\right)}(\hat{\rho}) = V^{\left(\frac{1}{2},\frac{1}{2}\right)}(\hat{\rho}) = \left(\left\langle \frac{1}{2}\{\hat{T}_{\frac{1}{2},m}, \ \hat{T}_{\frac{1}{2},m'}\}\right\rangle\right) - \begin{pmatrix} \langle \hat{q}\rangle \\ \langle \hat{p}\rangle \end{pmatrix} \begin{pmatrix} \langle \hat{q}\rangle & \langle \hat{p}\rangle \end{pmatrix}$$

$$= \begin{pmatrix} (\Delta q)^2 & \Delta(q,p) \\ \Delta(q,p) & (\Delta p)^2 \end{pmatrix} ;$$

$$\omega^{\left(\frac{1}{2}\right)}(\hat{\rho}) = \omega^{\left(\frac{1}{2},\frac{1}{2}\right)}(\hat{\rho}) = -i\begin{pmatrix} 0 & [\hat{q}, \hat{p}] \\ [\hat{p}, \hat{q}] & 0 \end{pmatrix} = i\hbar\sigma_2 ;$$

$$\tilde{\Omega}^{\left(\frac{1}{2}\right)}(\hat{\rho}) \geq 0 \quad \Leftrightarrow \quad \begin{pmatrix} (\Delta q)^2 & \Delta(q,p) + i\frac{\hbar}{2} \\ \Delta(q,p) - i\frac{\hbar}{2} & (\Delta p)^2 \end{pmatrix} \geq 0 \Leftrightarrow$$

$$(\Delta q)^2 (\Delta p)^2 - (\Delta(q,p))^2 \geq \frac{\hbar^2}{4}, \tag{4.29}$$

the original Schrödinger-Robertson UP.

It is natural to ask for the new conditions that appear at each step in the hierarchy (4.28), in passing from J to $J + \frac{1}{2}$. In the generic case, when we have a strict inequality we can find the answer using Lemma 1 of Section II. Comparing $\tilde{\Omega}^{\left(J+\frac{1}{2}\right)}(\hat{\rho})$ and $\tilde{\Omega}^{(J)}(\hat{\rho})$, in the notation of Eq. (2.10) and using Eq. (4.27) we have:

$$\tilde{\Omega}^{\left(J+\frac{1}{2}\right)}(\hat{\rho}) = \begin{pmatrix} A & C^\dagger \\ C & B \end{pmatrix} ;$$

$$A = \tilde{\Omega}^{(J)}(\hat{\rho}), \quad B = \tilde{\Omega}^{\left(J+\frac{1}{2},J+\frac{1}{2}\right)}(\hat{\rho}),$$

$$C = \left(\tilde{\Omega}^{\left(J+\frac{1}{2},\frac{1}{2}\right)}(\hat{\rho}) \ \cdots \ \tilde{\Omega}^{\left(J+\frac{1}{2},J\right)}(\hat{\rho})\right). \tag{4.30}$$

The 'dimensions' are $N_J \times N_J$, $2(J+1) \times 2(J+1)$, $2(J+1) \times N_J$ respectively. Then

$$\tilde{\Omega}^{\left(J+\frac{1}{2}\right)}(\hat{\rho}) > 0 \ \Leftrightarrow \ \tilde{\Omega}^{(J)}(\hat{\rho}) > 0, \ \ B - CA^{-1}C^\dagger > 0, \tag{4.31}$$

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where A, B, C are taken from Eq. (4.30). One can see that some complication arises from the need to compute A^{-1} in the new condition.

In the next Section, we analyse the case $J = \frac{1}{2} \to J + \frac{1}{2} = 1$ in some detail, as the first nontrivial step going beyond the Schrödinger-Robertson UP (3.7, 4.29). Before we turn to this task, however, a note on the non-generic case of singular A seems to be in order.

Remark: Lemma 1 expresses the positive definiteness of a hermitian matrix Q in the block form (2.10) in terms of conditions on the lower dimensional blocks. The block form itself is a description of Q with respect to a given breakup of the underlying vector space on which Q acts, into two mutually orthogonal subspaces. Both A and B are hermitian. For the case of positive semidefinite Q, there are two possibilities at the level of A, B, C. If A^{-1} exists, then $Q \geq 0$ translates into $A > 0$, $B - C\,A^{-1}\,C^\dagger \geq 0$. In case A is singular, while of course $Q \geq 0$ implies $A \geq 0$, the question is what other condition on B, C is implied. To answer this, we further separate the subspace on which A acts into two mutually orthogonal subspaces—one corresponding to the null subspace of A, and the other on which A acts invertibly, say as A_1. Then in such a description, the block form of Q is initially refined to the form

$$
Q \simeq \begin{pmatrix} 0 & 0 & C_2^\dagger \\ 0 & A_1 & C_1^\dagger \\ C_2 & C_1 & B \end{pmatrix},
\tag{4.32}
$$

with the original A and C being respectively $\begin{pmatrix} 0 & 0 \\ 0 & A_1 \end{pmatrix}$ and $(C_2,\, C_1)$. But now one sees easily that $Q \geq 0$ implies $C_2 = 0$, so as A_1^{-1} exists, we have in this situation

$$
Q \geq 0 \quad \Leftrightarrow \quad A_1 > 0, \ \ B - C_1\,A_1^{-1}\,C_1^\dagger \geq 0.
\tag{4.33}
$$

This is the description of the nongeneric situation mentioned above.

V. $SO(2,1)$ **ANALYSIS OF FOURTH ORDER MOMENTS**

The first nontrivial step in the hierarchy of uncertainty relations (4.28), after the Schrödinger-Robertson UP (3.7, 4.29), occurs in going from $J = \frac{1}{2}$ to $J + \frac{1}{2} = 1$. We study this in some detail, especially as it brings into evidence the equivalence of the irreducible representation $K^{(1)}(S)$ of $Sp(2,\,R)$ and the defining representation of the three-dimensional

proper homogeneous Lorentz group $SO(2,1)$ [26]. Indeed $K^{(2)}(S)$, $K^{(3)}(S)$, $\cdots$ are all true representations of $SO(2,1)$ [27].

It is useful to introduce specific symbols for the operators $\hat{T}_{\frac{1}{2}m}$, $\hat{T}_{1m}$ in the present context. We write

$$(\hat{T}_{\frac{1}{2}m}) = (\hat{\xi}_m) = \begin{pmatrix} \hat{q} \\ \hat{p} \end{pmatrix}, \quad m = \frac{1}{2}, -\frac{1}{2};$$

$$(\hat{T}_{1m}) = (\hat{X}_m) = \begin{pmatrix} \hat{q}^2 \\ \frac{1}{2}\{\hat{q}, \hat{p}\} \\ \hat{p}^2 \end{pmatrix}, \quad m = 1, 0, -1; \tag{5.1}$$

so that one immediately recognises that $\hat{\xi}$ is a two-component spinor, and $\hat{X}$ a three-component vector, with respect to $SO(2,1)$ (see below). Their products can be computed using Eq. (4.16) or more directly by simple algebra:

$$\begin{aligned}
\hat{\xi}_m \, \hat{\xi}_{m'} &= \hat{X}_{m+m'} + i\, \tfrac{\hbar}{2}(-1)^{m-\frac{1}{2}}\, \delta_{m+m',0}; & (a) \\
\hat{\xi}_m \, \hat{X}_{m'} &= \hat{T}_{\frac{3}{2},\, m+m'} + i\, \tfrac{\hbar}{2}(-1)^{m-\frac{1}{2}}\, \hat{\xi}_{m+m'}; & (b) \\
\hat{X}_m \, \hat{X}_{m'} &= \hat{T}_{2,\, m+m'} + \tfrac{\hbar^2}{4}(-1)^m\,(1+m^2)\,\delta_{m+m',0} + i\,\hbar\,(m-m')\,\hat{X}_{m+m'}. & (c)
\end{aligned} \tag{5.2}$$

In (5.2a) the leading $J = 1$ term is symmetric in m, m'; while the pure imaginary $J = 0$ second term is antisymmetric. In (5.2b) it is understood that $\hat{\xi}_{\pm\frac{3}{2}} = 0$. In (5.2c) the first two $J = 2$ and $J = 0$ terms are symmetric in m, m'; while the third $J = 1$ term is antisymmetric. These features agree with the pattern in Eq. (4.22).

For $J = \frac{1}{2}$ in Eq. (4.30) we have

$$A = \tilde{\Omega}^{\left(\frac{1}{2}, \frac{1}{2}\right)}(\hat{\rho}), \quad B = \tilde{\Omega}^{(1, 1)}(\hat{\rho}), \quad C = \tilde{\Omega}^{\left(1, \frac{1}{2}\right)}(\hat{\rho}), \tag{5.3}$$

with 'dimensions' 2×2, 3×3, 3×2 respectively. (Throughout this Section, A, B, C will have these meanings). Their behaviours under $Sp(2, R)$ are

$$\hat{\rho} \to \hat{\rho}' = \overline{U}(S)\, \hat{\rho}\, \overline{U}(S)^{-1} \Rightarrow A \to S\, A\, S^T, \quad B \to K^{(1)}(S)\, B\, K^{(1)}(S)^T,$$

$$C \to K^{(1)}(S)\, C\, S^T. \tag{5.4}$$

Assuming A^{-1} exists, we have

$$A^{-1} \to (S^{-1})^T\, A^{-1}\, S^{-1}, \tag{5.5}$$

and consequently,

$$B - C\,A^{-1}\,C^\dagger \to K^{(1)}(S)\,(B - C\,A^{-1}\,C^\dagger)\,K^{(1)}(S)^T, \tag{5.6}$$

which as expected is a congruence.

The matrix $K^{(1)}(S)$ is easily found. At the level of classical variables:

$$S = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in Sp(2,\,R): \quad \begin{pmatrix} q \\ p \end{pmatrix} \to S \begin{pmatrix} q \\ p \end{pmatrix} \Rightarrow$$

$$(X_m(q,\,p)) = \begin{pmatrix} q^2 \\ qp \\ p^2 \end{pmatrix} \to K^{(1)}(S)\,(X_m(q,p)),$$

$$K^{(1)}(S) = \begin{pmatrix} a^2 & 2ab & b^2 \\ ac & ad+bc & bd \\ c^2 & 2cd & d^2 \end{pmatrix}. \tag{5.7}$$

The link to $SO(2,1)$ can be seen in two (essentially equivalent) ways, either through A or through $(X_m(q,p))$. We now outline both.

We introduce indices μ, ν, $\cdots$ going over values 0, 3, 1 (in that sequence) and a three-dimensional Lorentz metric $g_{\mu\nu} = \mathrm{diag}(+1,\,-1,\,-1)$. This metric and its inverse $g^{\mu\nu}$ are used for lowering and raising Greek indices. The defining representation of the proper homogeneous Lorentz group $SO(2,1)$ is then:

$$SO(2,1) = \{\Lambda = (\Lambda^\mu{}_\nu) = 3 \times 3 \text{ real matrix} \mid \Lambda^\mu{}_\nu\,\Lambda_{\mu\lambda} \equiv g_{\mu\tau}\,\Lambda^\mu{}_\nu\,\Lambda^\tau{}_\lambda = g_{\nu\lambda},$$

$$\det \Lambda = +1,\ \ \Lambda^0{}_0 \ge 1\}. \tag{5.8}$$

This is a three-parameter noncompact Lie group. Now expand $A = \tilde{\Omega}^{\left(\frac{1}{2},\frac{1}{2}\right)}(\hat{\rho})$ in terms of Pauli matrices as follows:

$$A = \tilde{\Omega}^{\left(\frac{1}{2},\frac{1}{2}\right)}(\hat{\rho}) = x^\mu\,\sigma_\mu - \frac{\hbar}{2}\sigma_2 = \begin{pmatrix} x^0 + x^3 & x^1 \\ x^1 & x^0 - x^3 \end{pmatrix} - \frac{\hbar}{2}\sigma_2. \tag{5.9}$$

From Eqs. (3.6, 4.29) we have (indicating $\hat{\rho}$ dependences):

$$x^0(\hat{\rho}) = \frac{1}{2}((\Delta q)^2 + (\Delta p)^2),\ \ x^3(\hat{\rho}) = \frac{1}{2}((\Delta q)^2 - (\Delta p)^2),\ \ x^1(\hat{\rho}) = \Delta(q,p) \tag{5.10}$$

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Then the transformation rule for A in Eq. (5.4), combined with $S\,\sigma_2\,S^T = \sigma_2$, leads to a rule for $x^\mu(\hat\rho)$:

$$\hat\rho \to \overline{U}(S)\,\hat\rho\,\overline{U}(S)^{-1} \;\Rightarrow\; A \to S\,A\,S^T \;\Rightarrow\; x^\mu(\hat\rho) \to \Lambda^\mu{}_\nu(S)\,x^\nu(\hat\rho),$$

$$\Lambda(S) = \begin{pmatrix} \frac{1}{2}(a^2 + b^2 + c^2 + d^2) & \frac{1}{2}(a^2 - b^2 + c^2 - d^2) & ab + cd \\ \frac{1}{2}(a^2 + b^2 - c^2 - d^2) & \frac{1}{2}(a^2 - b^2 - c^2 + d^2) & ab - cd \\ ac + bd & ac - bd & ad + bc \end{pmatrix} \in SO(2,1). \quad (5.11)$$

Thus $x^\mu(\hat\rho)$ transforms as a Lorentz three-vector, and the associated invariant is seen to be

$$x^\mu(\hat\rho)\,x_\mu(\hat\rho) = g_{\mu\nu}\,x^\mu(\hat\rho)\,x^\nu(\hat\rho) = (\Delta q)^2\,(\Delta p)^2 - (\Delta(q,p))^2 \geq \frac{\hbar^2}{4}, \quad (5.12)$$

so the Schrödinger-Robertson UP implies the geometrical statement that $x^\mu(\hat\rho)$ is positive time-like.

The matrices $K^{(1)}(S)$ by which $\hat{X}_m$ transform under $Sp(2,R)$ are related by a fixed similarity transform to the $\Lambda(S)$ above. If in terms of classical variables we pass from the components $X_m(q,p)$ in Eq. (5.7) to a new set of components $X^\mu(q,p)$ by

$$(X^\mu(q,p)) = \begin{pmatrix} \frac{1}{2}(q^2 + p^2) \\ \frac{1}{2}(q^2 - p^2) \\ qp \end{pmatrix} = M \begin{pmatrix} q^2 \\ qp \\ p^2 \end{pmatrix},$$

$$X^\mu(q,p) = M^\mu{}_m\,X_m(q,p), \quad X_m(q,p) = M^{-1}_{m\mu}\,X^\mu(q,p),$$

$$M = (M^\mu{}_m) = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \end{pmatrix}, \quad M^{-1} = (M^{-1}_{m\mu}) = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & -1 & 0 \end{pmatrix}, \quad (5.13)$$

then in place of Eq. (5.7) we have

$$\begin{pmatrix} q \\ p \end{pmatrix} \to S \begin{pmatrix} q \\ p \end{pmatrix} \;\Rightarrow\; X^\mu(q,p) \to M^\mu{}_m\,K^{(1)}_{mm'}(S)\,M^{-1}_{m'\nu}\,X^\nu(q,p)$$

$$= \Lambda^\mu{}_\nu(S)\,X^\nu(q,p),$$

$$K^{(1)}(S) = M^{-1}\,\Lambda(S)\,M. \quad (5.14)$$

At the operator level we have

$$\hat{X}^0 = \frac{1}{2}(\hat{q}^2 + \hat{p}^2), \quad \hat{X}^3 = \frac{1}{2}(\hat{q}^2 - \hat{p}^2), \quad \hat{X}^1 = \frac{1}{2}\{\hat{q},\,\hat{p}\},$$

$$\hat{X}^\mu = M^\mu{}_m\,\hat{X}_m, \quad (5.15)$$

and, as consequence of Eq. (4.14)), the twin equivalent transformation laws:

$$S \in Sp(2,\,R) \; : \;\; \overline{U}(S)^{-1}\,\hat{X}_m\,\overline{U}(S) = K^{(1)}_{mm'}(S)\,\hat{X}_{m'},$$

$$\overline{U}(S)^{-1}\,\hat{X}^\mu\,\overline{U}(S) = \Lambda^\mu{}_\nu(S)\,\hat{X}^\nu. \tag{5.16}$$

The upshot is that the matrices $K^{(1)}(S)$ are just the 'ordinary' homogeneous Lorentz transformation matrices $\Lambda(S)$ in a 'tilted' basis. The metric preserved by them is easily found though unfamiliar:

$$K^{(1)}(S)\,g_K\,K^{(1)}(S)^T = g_K,$$

$$g_K = M^{-1}\,g\,(M^{-1})^T = \begin{pmatrix} 0 & 0 & 2 \\ 0 & -1 & 0 \\ 2 & 0 & 0 \end{pmatrix}. \tag{5.17}$$

This enables us to use the nomenclature and geometrical features of three-dimensional Minkowski space even while working with operators $\hat{X}_m$ and transformation matrices $K^{(1)}(S)$.

Now we proceed to analyse the three matrices A, B, C and the combination $B - C\,A^{-1}\,C^\dagger$. (We have already parametrised A in Eqs. (5.9, 5.10)). Using Eqs. (5.2), their matrix elements are

$$A_{mm'} = \langle \hat{\xi}_m\,\hat{\xi}_{m'} \rangle - \langle \hat{\xi}_m \rangle\,\langle \hat{\xi}_{m'} \rangle$$

$$= \langle \hat{X}_{m+m'} \rangle - \langle \hat{\xi}_m \rangle\,\langle \hat{\xi}_{m'} \rangle + i\,\frac{\hbar}{2}\,(-1)^{m-\frac{1}{2}}\,\delta_{m,\,-m'}$$

$$= (x^\mu\,\sigma_\mu)_{mm'} + i\,\frac{\hbar}{2}\,(-1)^{m-\frac{1}{2}}\,\delta_{m,\,-m'} \, ;$$

$$B_{mm'} = \langle \hat{X}_m\,\hat{X}_{m'} \rangle - \langle \hat{X}_m \rangle\,\langle \hat{X}_{m'} \rangle$$

$$= \langle \hat{T}_{2,m+m'} \rangle + \frac{\hbar^2}{4}\,(-1)^m\,\delta_{m,-m'} - \langle \hat{X}_m \rangle\,\langle \hat{X}_{m'} \rangle + i\,\hbar\,(m-m')\,\langle \hat{X}_{m+m'} \rangle;$$

$$C_{mm'} = \langle \hat{X}_m\,\hat{\xi}_{m'} \rangle - \langle \hat{X}_m \rangle\,\langle \hat{\xi}_{m'} \rangle$$

$$= \langle \hat{T}_{\frac{3}{2},m+m'} \rangle - \langle \hat{X}_m \rangle\,\langle \hat{\xi}_{m'} \rangle - i\,\frac{\hbar}{2}\,(-1)^{m'-\frac{1}{2}}\,\langle \hat{\xi}_{m+m'} \rangle. \tag{5.18}$$

In each of these expressions, the possible values for m, m' are evident from the context. We now note an important fact in respect of the final forms of all three expressions: apart from explicit appearances of i in the last terms, *all other quantities are real.* This allows us to easily separate each of A, B, C into real and imaginary parts, which in the cases of A and B are respectively symmetric and antisymmetric in m and m'. [This is already seen in

Eq. (5.9) for A]. We write these as follows:

$$A = A_1 + i\, A_2,$$

$$(A_1)_{mm'} = \langle \hat{X}_{m+m'}\rangle - \langle \hat{\xi}_m\rangle\, \langle \hat{\xi}_{m'}\rangle = (x^\mu\, \sigma_\mu)_{mm'},$$

$$(A_2)_{mm'} = \tfrac{\hbar}{2}(-1)^{m-\frac{1}{2}}\, \delta_{m,\,-m'}; \qquad (a)$$

$$B = B_1 + i\, B_2,$$

$$(B_1)_{mm'} = \langle \hat{T}_{2,m+m'}\rangle + \tfrac{\hbar^2}{4}(-1)^m\, \delta_{m,-m'} - \langle \hat{X}_m\rangle\, \langle \hat{X}_{m'}\rangle,$$

$$(B_2)_{mm'} = \hbar\,(m - m')\, \langle \hat{X}_{m+m'}\rangle; \qquad (b)$$

$$C = C_1 + i\, C_2;$$

$$(C_1)_{mm'} = \langle \hat{T}_{\frac{3}{2},m+m'}\rangle - \langle \hat{X}_m\rangle\, \langle \hat{\xi}_{m'}\rangle,$$

$$(C_2)_{mm'} = -\tfrac{\hbar}{2}(-1)^{m'-\frac{1}{2}}\, \langle \hat{\xi}_{m+m'}\rangle;$$

$$C^\dagger = C_1^T - i\, C_2^T. \qquad (c)$$

$$(5.19)$$

To deal similarly with $B - C\,A^{-1}\,C^\dagger$, we need an expression for A^{-1}. We will assume the generic situation in which A is nonsingular,

$$\det A \equiv \kappa^{-1} = x^\mu\, x_\mu - \frac{\hbar^2}{4} > 0, \qquad (5.20)$$

so that

$$A^{-1} = \kappa\big(x^0 - x^3\sigma_3 - x^1\sigma_1 + \frac{\hbar}{2}\,\sigma_2\big)$$

$$= \kappa\big(\tilde{x}^\mu\,\sigma_\mu + \frac{\hbar}{2}\,\sigma_2\big),$$

$$\tilde{x}^\mu = (x^0,\, -x^3,\, -x^1). \qquad (5.21)$$

The transformation law for A^{-1} under $S \in Sp(2, R)$ given in Eq. (5.5) is different from (though equivalent to) the law for A. Thus, while the $\tilde{x}^\mu$ do follow a definite (i.e., well defined tensorial [26]) transformation law, there are some differences (in signs) compared to the law followed by x^μ. Clearly the two terms in Eq. (5.21) are, as they stand, the real symmetric and the pure imaginary antisymmetric parts of A^{-1}. We can now handle $B - C\,A^{-1}\,C^\dagger$ in the same manner as above:

$$B - C\,A^{-1}\,C^\dagger = B_1 + i\, B_2 - \kappa(C_1 + i\, C_2)\,\big(\tilde{x}\cdot\sigma + \frac{\hbar}{2}\,\sigma_2\big)\,(C_1^T - i\, C_2^T)$$

$$= V^{(\mathrm{eff})} + \frac{i}{2}\,\omega^{(\mathrm{eff})},$$

$$V^{(\mathrm{eff})} = B_1 - \kappa\big(C_1\,\tilde{x}\cdot\sigma\,C_1^T + C_2\,\tilde{x}\cdot\sigma C_2^T + i\,\frac{\hbar}{2}C_2\,\sigma_2\,C_1^T - i\,\frac{\hbar}{2}\,C_1\,\sigma_2\,C_2^T\big),$$

$$\frac{1}{2}\,\omega^{(\mathrm{eff})} = B_2 - \kappa\big(C_2\,\tilde{x}\cdot\sigma\,C_1^T - C_1\,\tilde{x}\cdot\sigma C_2^T - i\,\frac{\hbar}{2}C_1\,\sigma_2\,C_1^T - i\,\frac{\hbar}{2}\,C_2\,\sigma_2\,C_2^T\big). \quad (5.22)$$

This decomposition is in the spirit and notation of Eq. (2.18) of the general framework. However, $V^{(\mathrm{eff})}$ and $\omega^{(\mathrm{eff})}$ do not correspond any longer to expectation values of simple anticommutators and commutators among relevant operators, as was the case in Eqs. (2.18, 4.19, 4.21).

Both $V^{(\mathrm{eff})}$ and $\omega^{(\mathrm{eff})}$ are real three-dimensional matrices with elements $V^{(\mathrm{eff})}_{mm'}$, $\omega^{(\mathrm{eff})}_{mm'}$, where $m, m' = 1, 0, -1$; and they are respectively symmetric and antisymmetric. It does not seem possible to simplify the expressions (5.22) to any significant extent, as they are already expressed in terms of the independent real expectation values $\langle \hat{\xi}_m \rangle$, $\langle \hat{X}_m \rangle$, $\langle \hat{T}_{\frac{3}{2},m} \rangle$, $\langle \hat{T}_{2,m} \rangle$ which are the moments of the Wigner distribution $W(q, p)$ of orders up to and including the fourth. Under action by $S \in Sp(2, R)$ we have from Eq. (5.6):

$$\hat{\rho} \to \overline{U}(S)\, \hat{\rho}\, \overline{U}(S)^{-1} \;\Rightarrow\; V^{(\mathrm{eff})} \to K^{(1)}(S)\, V^{(\mathrm{eff})}\, K^{(1)}(S)^T,$$
$$\omega^{(\mathrm{eff})} \to K^{(1)}(S)\, \omega^{(\mathrm{eff})}\, K^{(1)}(S)^T. \tag{5.23}$$

The added uncertainty relation up to the fourth order going beyond the Schrödinger-Robertson UP (3.7, 4.29), reads [in the generic case $\det A > 0$]:

$$V^{(\mathrm{eff})} + \frac{i}{2}\, \omega^{(\mathrm{eff})} \geq 0, \tag{5.24}$$

which is an $SO(2,1)$ covariant statement by virtue of Eq. (5.23).

For further analysis it is rather awkward to work with $SO(2,1)$ matrices and Lorentz metric in the form $K^{(1)}(S)$, g_K, therefore we pass to the 'standard' forms via the matrices M, M^{-1} in Eq. (5.13):

$$V^{(\mathrm{eff})\,\mu\nu} = M^{\mu}{}_{m}\, M^{\nu}{}_{m'}\, V^{(\mathrm{eff})}_{mm'},$$
$$\omega^{(\mathrm{eff})\,\mu\nu} = M^{\mu}{}_{m}\, M^{\nu}{}_{m'}\, \omega^{(\mathrm{eff})}_{mm'}, \tag{5.25}$$

which are congruences. Then the $Sp(2, R)$ or $SO(2, 1)$ actions (5.23) appear as:

$$V^{(\mathrm{eff})\,\mu\nu} \to \Lambda^{\mu}{}_{\mu'}(S)\, \Lambda^{\nu}{}_{\nu'}(S)\, V^{(\mathrm{eff})\,\mu'\nu'},$$
$$\omega^{(\mathrm{eff})\,\mu\nu} \to \Lambda^{\mu}{}_{\mu'}(S)\, \Lambda^{\nu}{}_{\nu'}(S)\, \omega^{(\mathrm{eff})\,\mu'\nu'}, \tag{5.26}$$

and the condition (5.24) becomes:

$$(V^{(\mathrm{eff})\,\mu\nu}) + \frac{i}{2}\, (\omega^{(\mathrm{eff})\,\mu\nu}) \geq 0. \tag{5.27}$$

While $V^{(\mathrm{eff})\,\mu\nu}$ transforms as a symmetric second rank $SO(2,1)$ tensor, $\omega^{(\mathrm{eff})\,\mu\nu}$ is an anti-symmetric second rank tensor, which by the use of the Levi Civita invariant tensor is the same as a three vector. Thus we can write, with $\epsilon^{031} = \epsilon_{031} = +1$,

$$\omega^{(\mathrm{eff})\,\mu\nu} = \epsilon^{\mu\nu\lambda}\, a_\lambda,$$

$$(\omega^{(\mathrm{eff})\,\mu\nu}) = \begin{pmatrix} 0 & a_1 & -a_3 \\ -a_1 & 0 & a_0 \\ a_3 & -a_0 & 0 \end{pmatrix}, \tag{5.28}$$

with transformation law

$$a^\mu \to \Lambda^\mu{}_\nu(S)\, a^\nu. \tag{5.29}$$

Of course, $V^{(\mathrm{eff})\,\mu\nu}$ itself is made up of two irreducible parts: the symmetric second rank 'trace-free' part belonging to the $SO(2,1)$ representation $K^{(2)}(S)$, and the $SO(2,1)$ invariant trace which is a scalar.

We now appeal to a remarkable result [22], which is similar in spirit to the Williamson theorem for $Sp(2n,R)$ quoted in Section 3. It states that if $V^{(\mathrm{eff})\,\mu\nu}$ transforming as in Eq. (5.26) is positive definite, it is possible to bring it to a diagonal form by a suitable choice of $\Lambda \in SO(2,1)$; however in general the resulting diagonal values are not the eigenvalues of the initial matrix. This diagonal form may be called the 'SCS normal form' of $V^{(\mathrm{eff})}$, which in the generic case is unique. Passing to this normal form of $V^{(\mathrm{eff})}$, and transforming $\omega^{(\mathrm{eff})}$ as well by the same (generically unique) $\Lambda \in SO(2,1)$, these matrices appear as

$$V^{(\mathrm{eff})} \to \begin{pmatrix} v^{00} & 0 & 0 \\ 0 & v^{33} & 0 \\ 0 & 0 & v^{11} \end{pmatrix}, \quad \omega^{(\mathrm{eff})} \to \begin{pmatrix} 0 & -b^1 & b^3 \\ b^1 & 0 & b^0 \\ -b^3 & -b^0 & 0 \end{pmatrix}, \tag{5.30}$$

with all the quantities v^{00}, v^{33}, v^{11}, b^0, b^3, b^1 being real $SO(2,1)$ (and $Sp(2,R)$) invariants. The uncertainty relation (5.27) expressed in terms of these invariants, and in its maximally simplified form thanks to the SCS theorem, is

$$\begin{pmatrix} v^{00} & 0 & 0 \\ 0 & v^{33} & 0 \\ 0 & 0 & v^{11} \end{pmatrix} + \frac{i}{2}\begin{pmatrix} 0 & -b^1 & b^3 \\ b^1 & 0 & b^0 \\ -b^3 & -b^0 & 0 \end{pmatrix} \geq 0. \tag{5.31}$$

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As an (admittedly elementary) example of the discussion of this Section, we consider the Fock states $|n\rangle$, $n \geq 0$. The $(\hat{q}, \hat{p}) - (\hat{a}, \hat{a}^\dagger)$ relations are

$$\hat{a} = (\hat{q} + i\hat{p})/\sqrt{2\hbar}, \quad \hat{a}^\dagger = (\hat{q} - i\hat{p})/\sqrt{2\hbar}, \tag{5.32}$$

so both $\hat{q}$ and $\hat{p}$ have dimensions $\hbar^{1/2}$. In the Fock states $|n\rangle$, by parity arguments we have

$$\langle n|\hat{\xi}_m|n\rangle = \langle n|\hat{T}_{3/2,m}|n\rangle = 0. \tag{5.33}$$

For $\hat{X}_m$, $\hat{T}_{2,m}$ explicit calculations give:

$$\langle n|\hat{X}_m|n\rangle = \hbar(n + \tfrac{1}{2})(1, \, 0, \, 1), \quad m = 1, \, 0, \, -1;$$

$$\langle n|\hat{T}_{2,m}|n\rangle = \frac{1}{2}\hbar^2(n^2 + n + \tfrac{1}{2})(3, \, 0, \, 1, \, 0, \, 3), \quad m = 2, \, 1, \, 0, \, -1, \, -2. \tag{5.34}$$

Then the matrices A, B, C of Eq. (5.3) follow easily:

$$(A_{mm'}) = \hbar(n + \tfrac{1}{2})\mathbb{1} - \tfrac{\hbar}{2}\sigma_2,$$
$$x^0 = \hbar(n + \tfrac{1}{2}), \quad x^3 = x^1 = 0; \tag{a}$$

$$(B_{mm'}) = \tfrac{\hbar^2}{2}(n^2 + n + 1)\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} + i\hbar^2(n + \tfrac{1}{2})\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}; \quad (b) \tag{5.35}$$

$$(C_{mm'}) = 0. \tag{c}$$

Therefore the combination $B - CA^{-1}C^\dagger = B$, and from Eq. (5.22),

$$\left(V_{mm'}^{(\text{eff})}\right) = \frac{\hbar^2}{2}(n^2 + n + 1)\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix},$$

$$\frac{1}{2}\left(\omega_{mm'}^{(\text{eff})}\right) = \hbar^2(n + \tfrac{1}{2})\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}. \tag{5.36}$$

Transforming to the standard $SO(2,1)$ tensor components by the congruence transforma-

tion (5.25) we find:

$$
\left(V^{(\text{eff})\,\mu\nu}\right) = \frac{\hbar^2}{2}(n^2 + n + 1)
\begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix},
$$

$$
\frac{1}{2}\left(\omega^{(\text{eff})\,\mu\nu}\right) = \hbar^2(n + \tfrac{1}{2})
\begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & -1 & 0
\end{pmatrix}. \tag{5.37}
$$

As expected, both these matrices are invariant under the $SO(2)$ subgroup of $SO(2, 1)$, as the Fock states are eigenstates of the phase space rotation generator $\hat{a}^\dagger \hat{a}$.

We see that $\left(V^{(\text{eff})\,\mu\nu}\right)$ is already in the SCS normal form, and as the eigenvalues of $\left(V^{(\text{eff})\,\mu\nu}\right) + \frac{i}{2}\left(\omega^{(\text{eff})\,\mu\nu}\right)$ are 0, $\frac{\hbar^2}{2}(n^2 + n + 1) \pm \hbar^2(n + \frac{1}{2})$, i.e., 0, $\frac{\hbar^2}{2}(n+1)(n+2)$, $\frac{\hbar^2}{2}n(n-1)$, the uncertainty relation (5.27) is clearly respected; indeed it is saturated!

VI.   LORENTZ GEOMETRY AND THE SCHRÖDINGER-ROBERTSON UP

The original Schrödinger-Robertson UP has a very interesting character when viewed in the Wigner distribution language, bringing out the role of the group $SO(2, 1)$ in a rather striking manner. This seems worth exploring in some detail.

For a given state $\hat{\rho}$ with Wigner distribution $W(q, p)$, the means are

$$
\overline{q} = \int\int dq\,dp\, q\, W(q,\, p)\,, \quad \overline{p} = \int\int dq\,dp\, p\, W(q,\, p)\,. \tag{6.1}
$$

Referring to Eq. (5.13), at each point (q, p) in the phase plane we define the $SO(2, 1)$ three-vector (a displaced form of $(X^\mu(q,p))$ in Eq. (5.13))

$$
(\,X^\mu(q,\, p)\,) =
\begin{pmatrix}
\frac{1}{2}\left[(q - \overline{q})^2 + (p - \overline{p})^2\right] \\
\frac{1}{2}\left[(q - \overline{q})^2 - (p - \overline{p})^2\right] \\
(q - \overline{q})(p - \overline{p})
\end{pmatrix}, \tag{6.2}
$$

which (except at $q = \overline{q}$, $p = \overline{p}$) is pointwise positive light-like. The elements of the variance matrix V in Eqs. (3.6, 4.29) are obtained by 'averaging' this three-vector over the phase plane with the quasiprobability $W(q,p)$ as 'weight' function, resulting in the three-vector

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$x^\mu(\hat{\rho})$ of Eq. (5.10) :

$$(x^\mu(\hat{\rho})) = \begin{pmatrix} \frac{1}{2}\left[(\triangle q)^2 + (\triangle p)^2\right] \\ \frac{1}{2}\left[(\triangle q)^2 - (\triangle p)^2\right] \\ \triangle(q,p) \end{pmatrix} = \int\int dq\,dp\, W(q,p)\,(X^\mu(q,p)). \qquad (6.3)$$

Given that $W(q,p)$ can in principle be negative over certain regions of the phase space, this 'averaging' could have led to a result which need not be either time-like or light-like positive. However the Schrödinger-Robertson UP assures us that in fact the result has to be a time-like positive three-vector, thus implying a subtle limit on the extent to which $W(q,p)$ could become negative. In fact it specifies that the three-vector obtained as a result of the 'averaging' must be within or on the positive time-like (solid) hyperboloid $\sum_\mu x^\mu(\hat{\rho})x_\mu(\hat{\rho}) \geq \hbar^2/4$ corresponding to 'squared mass' $\hbar^2/4$ presented in Eq. (5.12). On the other hand, while pointwise nonnegativity of $W(q,p)$ will certainly ensure that the averaging in Eq. (6.3) takes $(x^\mu(\hat{\rho}))$ inside the time-like positive cone, it will not itself ensure that it is taken all the way inside the said hyperboloid. To ensure the latter, $W(q,p)$ should have a threshold effective spread. Thus, pointwise nonnegativity is neither a necessary nor sufficient requirement to ensure 'Wigner quality' on $W(q,p)$ as is known from other considerations.

The argument above has been presented in such a way that the interpretation in terms of Lorentz geometry in $2+1$ dimensions is obvious. However, comparing Eqs. (5.7) and (5.13), we see that it could be expressed equally well as follows. At each point (q,p) in the phase plane we define a 2×2 real symmetric matrix

$$V(q,p) = \begin{pmatrix} q - \overline{q} \\ p - \overline{p} \end{pmatrix} \begin{pmatrix} q - \overline{q} & p - \overline{p} \end{pmatrix}. \qquad (6.4)$$

Pointwise (except at $q = \overline{q}$, $p = \overline{p}$) this is proportional to a one-dimensional projection matrix, and in particular it has vanishing determinant. After 'averaging' with $W(q,p)$ as weight function, however, we obtain the 2×2 variance matrix V in Eq. (4.29) :

$$V = \int\int dp\,dq\, W(q,p)V(q,p) = \begin{pmatrix} (\triangle q)^2 & \triangle(q,p) \\ \triangle(q,p) & (\triangle p)^2 \end{pmatrix}, \qquad (6.5)$$

and now the Schrödinger-Robertson UP shows that V is non-singular and has determinant bounded below by the 'squared mass' $\hbar^2/4$.

In this form, just like the Schrödinger-Robertson UP, this geometrical picture based on the Wigner distribution language generalises in both directions—second order moments for

a multi mode system, and higher order moments for a single mode system. As an example of the former, consider a two-mode system for simplicity. The classical phase space variables are ξ_a and the hermitian quantum operators obeying Eq. (3.1) are $\hat{\xi}_a$, for $a = 1, \cdots, 4$. Given a two-mode state $\hat{\rho}$, we pass to its Wigner distribution $W(\xi)$ (something we did not do in Section III) and compute the means

$$\langle \hat{\xi}_a \rangle = \mathrm{Tr}(\hat{\rho}\,\hat{\xi}_a) = \int d^4\xi\,\xi_a W(\xi) = \overline{\xi}_a, \; a = 1, \cdots, 4. \tag{6.6}$$

Then, generalising Eq. (6.4) above, at each point ξ in the 4-dimensional phase space we define a real symmetric 4×4 matrix

$$V(\xi) = (V_{ab}(\xi)) = ((\xi_a - \overline{\xi}_a)(\xi_b - \overline{\xi}_b)) = x(\xi)x(\xi)^T,$$
$$x_a(\xi) = \xi_a - \overline{\xi}_a. \tag{6.7}$$

At each point ξ (except at $\xi = \overline{\xi}$) we have here a real symmetric positive semidefinite matrix $V(\xi)$ which is essentially a one-dimensional projection matrix: the eigenvalues of $V(\xi)$ are $x(\xi)^T x(\xi), 0, 0, 0$. The variance matrix V for the state $\hat{\rho}$ is then obtained by 'averaging' $V(\xi)$ using the real normalised quasiprobability $W(\xi)$:

$$V = \int d^4\xi\, W(\xi)V(\xi). \tag{6.8}$$

Since in general $W(\xi)$ can assume negative values at some places in phase space, it may appear at first sight that some of the properties of $V(\xi)$ described above may be lost by the 'averaging' process leading to V. However the UP (3.5) guarantees that this will not happen; indeed by Lemma 2, Section II, in Eq. (2.13), V is seen to be positive definite. Quantitatively we have the following situation: Williamson's theorem assures us that under the congruence transformation by a suitable $S_0 \in Sp(4, \mathcal{R})$, V is taken to a diagonal form:

$$V_0 = S_0 V S_0^T = diag(\kappa_1, \kappa_1, \kappa_2, \kappa_2), \quad \kappa_{1,2} > 0. \tag{6.9}$$

The congruence transformation becomes a similarity transformation on $V\beta^{-1}$ [13], since:

$$S \in Sp(4, \mathcal{R}) : V' = SVS^T \leftrightarrow V'\beta^{-1} = SV\beta^{-1}S^{-1}. \tag{6.10}$$

Applying this to the transition $V \to V_0$ we see that as

$$V_0\beta^{-1} = -i \begin{pmatrix} \kappa_1\sigma_2 & 0 \\ 0 & \kappa_2\sigma_2 \end{pmatrix}, \tag{6.11}$$

the eigenvalues of $iV\beta^{-1}$ are $\pm\kappa_1, \pm\kappa_2$; and the UP (3.5) ensures that $\kappa_{1,2} \geq \hbar/2$. The κ's themselves are determined, upto an interchange, by the $Sp(4, \mathcal{R})$ invariant traces

$$\mathrm{Tr}(V\beta^{-1})^2 = -2(\kappa_1^2 + \kappa_2^2),$$
$$\mathrm{Tr}(V\beta^{-1})^4 = 2(\kappa_1^4 + \kappa_2^4). \tag{6.12}$$

The manner in which the geometrical picture, and the constraint on the extent to which $W(\xi)$ can become negative, both generalise in going to the multi mode situation is now clear.

A qualitatively similar situation (even if algebraically more involved) obtains when we generalise in the other direction—to higher order moments for a single mode system, and their uncertainty relations handled in the Wigner distribution language. Limiting ourselves to the moments upto fourth order, we are concerned in the notation of Eq. (4.24) with the uncertainty relation

$$\tilde{\Omega}^{(1)}(\hat{\rho}) \geq 0 \tag{6.13}$$

contained in the hierarchy (4.28), and its rendering in the Wigner distribution language. Combining the notations of Sections II and V, we have a set of five real phase space functions $A_a(q, p)$, $a = 1, 2, \cdots, 5$, and their hermitian operator counterparts in the Weyl sense:

$$(A_a(q, p)) = (q, \ p, \ q^2, \ qp, \ p^2)^T;$$
$$(\hat{A}_a) = ((A_a(q, p))_W) = (\hat{q}, \ \hat{p}, \ \hat{q}^2, \ \frac{1}{2}\{\hat{q}, \hat{p}\}, \ \hat{p}^2)^T, \tag{6.14}$$

a listing of the components $\hat{\xi}_m$, $\hat{X}_m$. In a given state $\hat{\rho}$ with Wigner distribution $W(q, p)$ we have the means

$$\langle \hat{A}_a \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}_a) = \int\int dp\, dq\, W(q, p) A_a(q, p) = \overline{A}_a. \tag{6.15}$$

To calculate the elements of $\tilde{\Omega}^{(1)}(\hat{\rho})$ we need to deal with the products $\hat{A}_a \hat{A}_b$. For these, using Eq. (5.2) we find:

$$\hat{A}_a \hat{A}_b = (A_a(q, p) A_b(q, p))_W + (C_{ab}(q, p))_W,$$

$$(C_{ab}(q, p)) = \begin{pmatrix} 0 & \frac{i\hbar}{2} & 0 & \frac{i\hbar q}{2} & \frac{i\hbar p}{2} \\ -\frac{i\hbar}{2} & 0 & -\frac{i\hbar q}{2} & -\frac{i\hbar p}{2} & 0 \\ 0 & \frac{i\hbar q}{2} & 0 & i\hbar q^2 & -\frac{\hbar^2}{2} + 2i\hbar qp \\ -\frac{i\hbar q}{2} & \frac{i\hbar p}{2} & -i\hbar q^2 & \frac{\hbar^2}{4} & i\hbar p^2 \\ -\frac{i\hbar p}{2} & 0 & -\frac{\hbar^2}{2} - 2i\hbar qp & -i\hbar p^2 & 0 \end{pmatrix}. \tag{6.16}$$

(We note that the real symmetric part of the matrix $C(q,p)$ is $-\frac{\hbar^2}{4}g_K$ in the lower 3×3 block, where g_K is the tilted form of the $(2+1)$ Lorentz metric in Eq. (5.17)). With these ingredients and referring to the general structure (2.16) we have the expression for $\tilde{\Omega}^{(1)}(\hat{\rho})$ in the Wigner distribution language:

$$\tilde{\Omega}^{(1)}(\hat{\rho}) = \left(\tilde{\Omega}^{(1)}_{ab}(\hat{\rho})\right) = \left(\mathrm{Tr}(\hat{\rho}(\hat{A}_a - \langle\hat{A}_a\rangle)(\hat{A}_b - \langle\hat{A}_b\rangle))\right)$$

$$= \left(\mathrm{Tr}(\hat{\rho}\left((A_a(q,p)A_b(q,p))_W - \overline{A}_a\overline{A}_b + (C_{ab}(q,p))_W\right))\right)$$

$$= \int\int dp dq\, W(q,p)\left(x(q,p)x(q,p)^T + (C_{ab}(q,p))\right),$$

$$x(q,p)^T = (q - \overline{q},\, p - \overline{p},\, q^2 - \overline{q^2},\, qp - \overline{qp},\, p^2 - \overline{p^2}). \tag{6.17}$$

At each point (q,p) in the phase plane, we have essentially a one-dimensional projector $x(q,p)x(q,p)^T$, together with a five-dimensional hermitian matrix $(C_{ab}(q,p))$ with elements involving $\hbar$ and $\hbar^2$ terms. The uncertainty relation (6.13) demands that the phase plane 'average' of this expression (hermitian matrix) with $W(q,p)$ as weight function be nonnegative. After this 'averaging', the leading term is no longer a one-dimensional projector; moreover, the pure imaginary antisymmetric part coming from this part of $C(q,p)$ being singular, Lemma 2 of Section II does not apply to the real symmetric part of $\tilde{\Omega}^{(1)}(\hat{\rho})$. In any event, (6.13) again constrains the extent to which $W(q,p)$ can become negative.

VII.   CONCLUDING REMARKS

In this paper we have set up a systematic procedure to obtain covariant uncertainty relations for general quantum systems. It applies equally well to continuous variable systems and to systems described by finite-dimensional Hilbert spaces, and even to systems based on the tensor product of the two, and consists of two ingredients: the choice of a collection of observables, and the action of unitary symmetry operations on them. We have shown that the uncertainty relations are automatically covariant—preserved in content—under every symmetry operation.

We have applied this to two important special cases: the fluctuations and covariances in coordinates and momenta of an n-mode canonical system; and to the set of all hermitian operator 'monomials' in canonical variables $\hat{q}$, $\hat{p}$ of a single mode system. These are both generalisations of the Schrödinger-Robertson UP in two distinct directions. The latter generalisation has been treated for definiteness using the Wigner distribution method.

We hope to have set up a robust yet flexible formalism which can be applied to all quantum systems, in particular to composite, for instance bipartite, systems. In such a case, by judicious choices of the operator sets $\{\hat{A}_a\}$ of Section II, one can devise tests for entanglement, exhibiting covariance under corresponding local symmetry operations. If for a bipartite system the operator $\hat{\rho}^{\mathrm{PT}}$[28], arising from partial transpose of a physical state $\hat{\rho}$, violates any uncertainty relation, the presence of entanglement in $\hat{\rho}$ follows[29, 30]. A systematic analysis along these lines of higher order moments in the bipartite multi-mode case will be presented elsewhere, keeping in mind that our general methods are applicable for both discrete and continuous variable systems, and even to composite systems consisting of either or both types as subsystems.

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